Abstract No. voyl357

Direct Observation of Single Atom Dopants and Electrically Deactivating Defects

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Beamline(s): X15B

Progress towards understanding the inherent limitations on obtaining the highest free-carrier densities in *n*-type Si has been made with x-ray absorption and scanning transmission electron microscopy (STEM) measurements of 3D Sb-doped Si. The saturation of electrically active carriers at high dopant concentrations had been explained using a model in which *two* Sb dopant donor atoms interact to form particular structures containing 3-fold coordinated, electrically neutral dopants. Such donor-*pair* (*DP*) defects offered an alternative to the conventionally accepted defects containing 3 or 4 dopants surrounding a vacancy, i.e., Sb_3V and Sb_4V. Unlike these vacancy complexes, the *DP* defects were shown to be consistent with x-ray absorption data, and calculated electrical activities for 2D- and 3D-Sb doped Si systems based on the *DP* defect model agree well with experiment. This year, STEM data from a highly 3D-doped sample ([Sb] . 9×10^{20} cm^{-3}) have confirmed that paired dopants are indeed the dominant electrically deactivating defect configuration in *n*-doped Si. The STEM measurements lacked sufficient resolution, however, to rule out the possibility that these defects are not Sb_2V complexes (see figures). Efforts at refining simulations of the x-ray absorption data to distinguish between *DP*2 and Sb_2V defects have proved to be nondefinitive because they depend too sensitively on calculated atomic positions. Additional STEM measurements are planned for obtaining simultaneous electron detection at high and low collection angles, which should successfully differentiate the two different defect structures.

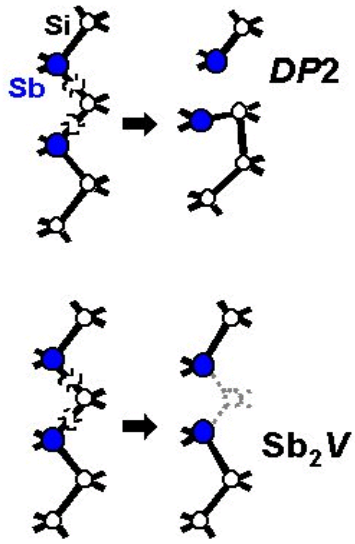

Figure 1. Schematic representation of two types of electrically deactivating defects in the Si(110) plane. Each contains a pair of 3-fold-coordinated, electrically neutral Sb atoms.

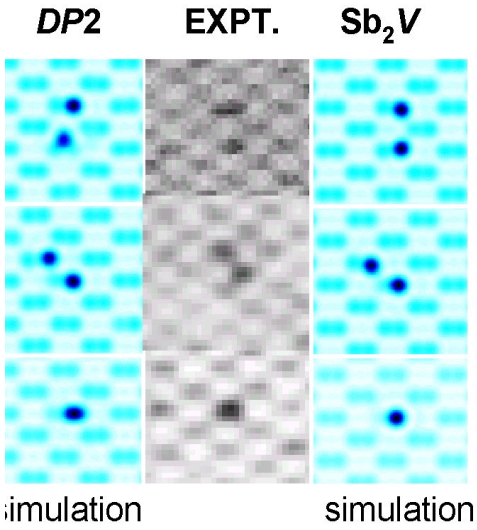

Figure 2. Comparison of STEM data with simulations of two types of electrically deactivating defects in the Si(110) plane. The present data cannot distinguish between the two defect structures.